User's Guide

SIMPAR

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User's Guide

SIMPAR

SIMPAR calculates the displacement of particles in a two-dimensional water flow environment.

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Contents

1 General directions for the use of SIMPAR

1.1 Background information

SIMPAR simulates the transport of floating particles and particles that behave like dissolved substances. It is an off-line program that calculates the movement of particles in two dimensions due to advection, diffusion and wind. Transport of particles by advection is based on a water movement model and is computed by interpolation fom the water velocities. SIMPAR uses the same grid as the water movement model.

In this section a concise mathematical description of SIMPAR is given. A more detailed description will be part of the technical documentation of SIMPAR.
The Directorate-General for Public Works and Water Management frequently uses transport models to calculate the effects of different discharging sources on surface waters. Policy plans and disasters may be computationally validated with it. Matter transport of different compositions may be simulated with the so called particle model. There are two possibilities for this particle model:
a random walk model or a fractional Brownian motion.
The particle model is based on a stochastic differential equation. The equation contains two parts, a drift part and a diffusion part. The drift part is related to the water flow and the bottom topography. The relevant data are given by the WAQUA water movement model in an SDS file. The diffusion part is a stochastic model: the particle makes random jumps in the direction of the water flow or in a direction perpendicular to it. The size of the jump is determined by chance.
In a random walk model the diffusion part is based on the Wiener process where the spreading of particles grow linearly with time.
In a fractional Brownian motion the diffusion part is based on the so called fractional Brownian motion where the spreading of particles varies in time. The user can choose either the random walk model or fractional Brownian motion for the simulation.

1.2 Rectilinear model

1.2.1 General

To model advection-diffusion the movement of a single particle is insignificant, but the movement of a large collection of particles undergoing drift and random motion, is significant. The displacement of a particle by drift is determined by a time integration of the WAQUA given flow velocity and the gradients of the bottom topography. The random displacement is based on the so called Wiener process, in which the particle undergoes a longitudinal (in the direction of flow) as well as a transversal deviation. To this end a random number is drawn for each direction from a probability distribution.

Instead of the Wiener process the random displacement can also be based on the fractional Brownian motion.

Some of the aspects are illustrated in Fig. 1.

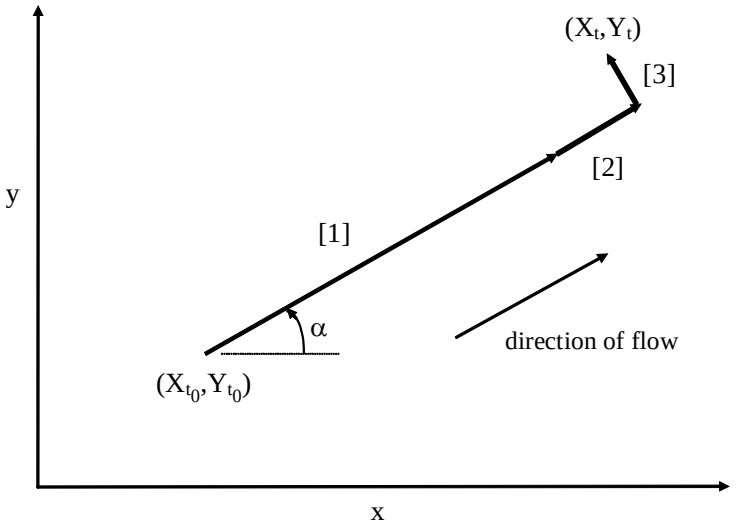


Fig. 1 Movement of a particle by advection and diffusion.

(X_{t_0},Y_{t_0}) position of the particle at time t_o
(X_t,Y_t) position of the particle at time t
[1] advection part
[2] diffusion part parallel to the flow direction
[3] diffusion part normal to the flow direction

1.2.2 Mathematical description

The position ☐ (see Fig. 1) in a cartesian coordinate system (x,y) of a particle, which at time t_0 is injected at position ☐, may be described by the so called stochastic differential equations:

(1) ☐

← drift part → ←——— diffusion part ———→

in which ☐, ☐ are independent components [2] and [3] of the Wiener process parallel to the direction of flow resp. normal to the direction of flow:

(2) ☐

☐

, and , are the so called components of the drift vector resp. the elements of the diffusion matrix:

(3)

(4)

← flow velocity → ← additional velocity caused by spatial variation of water depth and diffusion→

= total water depth till bottom
= depth mean velocity in x-direction
= depth mean velocity in y-direction
D = diffusion coefficient
= angle between direction of flow and x-axis

The first term in the driftvector components is the flow velocity. The second term in the driftvector components is an additional velocity as a consequence of spatial variation of water depth and diffusion.

1.2.2.1 The Wiener process

The equations (1) may be conceived as a symbolic notation of the next stochastic integral equations:

(5)

The position of the particle is a stochastic process, in which the probability density function for satisfies the following Fokker-Planck equation:

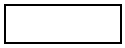
(6)

with initial condition:

(7)

A.W. Heemink has demonstrated (cf. Ref. 1), that there exists a relation between the probability density p satisfying the Fokker-Planck

equation and the concentration c in the Eulerian advection diffusion eqation, as used in WAQUA, namely:

(8) 

This means that the particle movement satisfies the Eulerian advection-diffusion equation, i.e. both models start from the same physical assumptions, the differences are only numerical in nature.

1.2.2.2 Fractional Brownian motion

The user can choose for the diffusion part to be based on the fractional Brownian motion in stead of the Wiener process. This choice is made by means of keyword **IHURST**. (see User Input)

…
…
…

When ½ < hurst factor < 1, the motion is *persistent*, meaning that the probability that a particle continues to move in the same direction it came from is large; the spreading of the particles is larger.
For hurstfactor = ½ , we have the random walk movement.
When 0 < hurst factor < ½ , the motion is *anti-persistent*, meaning that the probability that a particle will choose a different direction than the one it came from is increased; the spreading is smaller.

For more detailed information about concentration profiles see the report "The modeling of Diffusion in Particle Models" (cf. Ref. J.W. Stijnen, H.X.Lin (2000))

1.2.2.3 The rectilinear grid

The rectilinear grid on which SIMPAR makes its calculations, is furnished by WAQUA. It looks as follows (see User's Guide WAQUA)

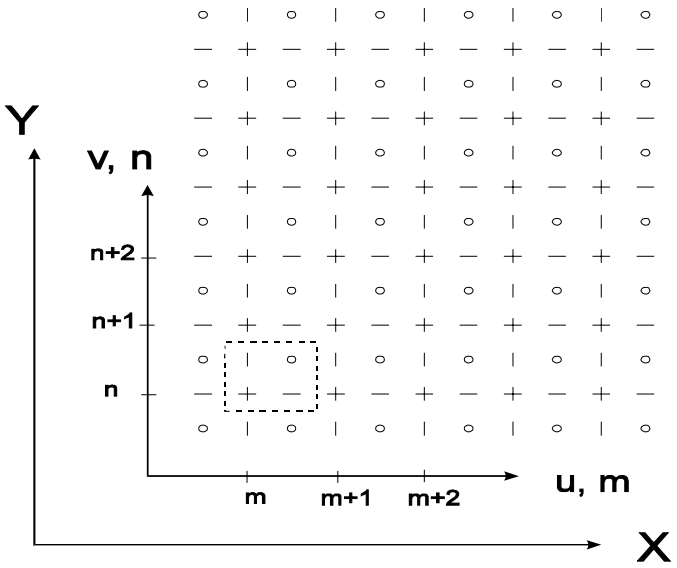


Fig. 2 Rectilinear grid

1.3 Curvilinear model

1.3.1 General

Curvilinear coordinates are frequently used in WAQUA for the simulation of water movement. This is an attempt to reflect the geometry as faithfully as possible and to introduce a local refinement. The calculations are performed in this case on a non-equidistant grid (cf. Fig. 3)

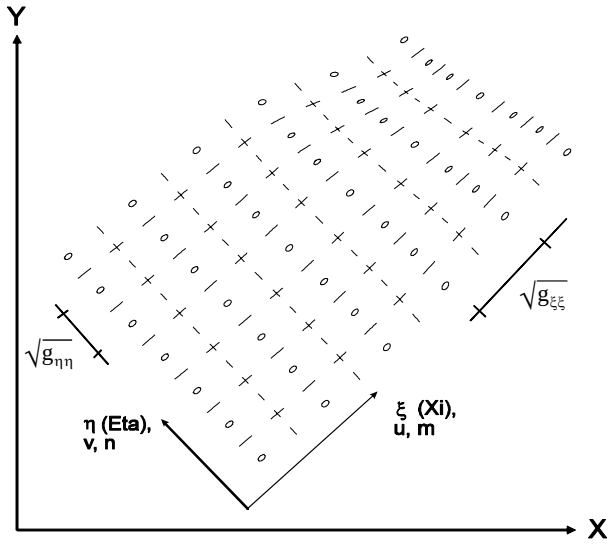


Fig. 3 Curvilineair grid

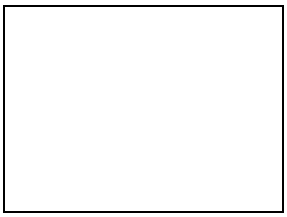
The curvilinear coordinates are denoted by [ ] and the cartesian coordinates by (x,y). A geometry in the cartesian (x,y)-plane, also called physical plane, is projected on the [ ] plane, the so called computational plane, by means of the following transformations:

(9)

The curves [ ]= constant and[ ]= constant build two systems of coordinate lines. WAQUA requires that these coordinate lines are orthogonal.

[ ] Are the transformation coefficients of the (x,y)-cartesian system to the [ ]-curvilinear system.

(10)

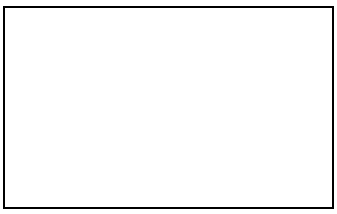


The curvilinear grid is furnished by WAQUA (in the SDS-file).

1.3.2 Coordinate transformation of the random walk model

When using a curvilinear grid, the mathematical equations have to be adapted.
The relations between the components of the water velocity [ ]in the (x,y)-plane and the components [ ]in the [ ]-plane are given by:

(11)



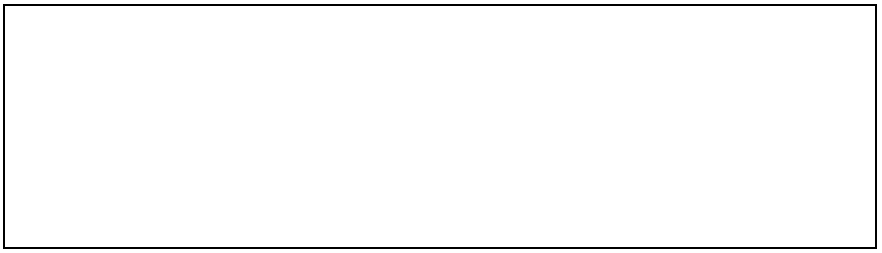
Substitution of the transformations gives the following equations of the random walk model:

(12)

← drift part → ←——— diffusion part ———→

in which:

(13)



← flow velocity → ← additional velocity caused by spatial variation of water depth and diffusion→

(14) $$G_{11} = \sqrt{\frac{2D}{g_{\xi\xi}}} \quad \text{and} \quad G_{22} = \sqrt{\frac{2D}{g_{\eta\eta}}}$$

□ = angle between the direction of flow and the local □ -direction

1.4 Boundary treatment in SIMPAR

1.4.1 Open boundaries:

When a particle passes an open bounary it is halted and removed from the calculations.

1.4.2 Closed boundaries:

When during the advective displacement the particle is about to pass a closed boundary, the calculation is renewed with half a timestep. This process is repeated, until the particle remains within the model area (see Fig. 4).

If during the random step the particle would cross the boundary, the particle is put back to its old position and a new random step is made. This procedure is repeated until the particle stays within the simulation area.

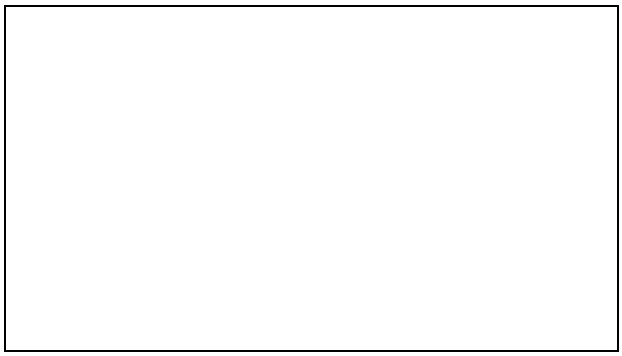


Fig. 4 Particle trajectory along the coast by halving the timestep

1.5 Dissolved versus floating transport

In SIMPAR an option is introduced to discern between ‘dissolved’ and ‘floating’ transport of a particle. The choice is made by means of the keyword IMODEL (see User Input). In the case of dissolved transport the spatial variation of the dispersion and the water depth is taken into account. This is reflected in the second term of the drift components in equations (13). In the case of floating transport it is not taken into account.

1.6 Involved files

SIMPAR utilizes it's own SDS files. In this file all necessary data is stored and will be used for postprocessing activities. A subset of this data has been generated by SIMPAR (e.g. position of particles) and another subset is copied from the WAQUA SDS file (e.g. geometry and water levels). WAQUA information that is actually used in a WAQUA computation, but not necessarily used for post processing purposes, is only read from a WAQUA SDS file but not copied.

1.7 Simulation time span

There are two cases to be considered:

- The simulation time span in SIMPAR and in WAQUA are identical and is called **the actual situation.** The displacement of particles as a result of advection in SIMPAR will be based on both momentaneous WAQUA velocities as well as Eulerian integrated velocities.

- The simulation time span in SIMPAR in a cyclic environment is a multiple of the WAQUA simulation time span . The WAQUA velocity fields (both momentaneous and integrated) can be used cyclically in order to calculate the displacement of particles as a consequence of advection. This facility has been introduced in order to make long term calculations.

1.8 Wind

In the Water Movement Model WAQUA the influence of wind on '**depth average'** velocities is taken into account. On behalf of the transport simulation of floating particles, a facility was created in order to provide an extra contribution of wind on the displacement of particles at the water surface. This is done by directly influencing the floating particles through a percentage of the wind velocity by means of a user defined factor.

Distinction between the following three cases can be made:

- Simulation of **dissolved** material:

The influence of wind on displacement of dissolved particles is already handled by displacement as a consequence of water movements. In a cyclic calculation it is impossible to work with an extra windfield within SIMPAR.

- Simulation of **floating** material using the actual wind fields of WAQUA:

The wind which is used by a WAQUA simulation and already has influenced the water movement, will be passed on to SIMPAR. The additional displacement of particles at the water surface by this wind is e qual to a factor times the wind speed times the timestep.

This factor is specified by the user.

Note:
In case of space varying wind, the wind can not be directly passed on to SIMPAR. Therefore the user has to specify a wind SDS-file, from which SIMPAR can obtain the needed wind values. It is the responsibility of the user that (s)he specifies the same wind SDS-file as used in WAQUA, because SIMPAR is unable to check this.

- Simulation of **floating** material combined with cyclical use of WAQUA fields within SIMPAR.

In the case of tidal water movements a varying wind may be used. While the wind in WAQUA is only available over a restricted period of time (a tide), this wind variation in time (but uniform in space) has to be introduced in SIMPAR by a time sequence of winds, or in case of space varying wind by a wind SDS-file. The wind driven displacement at the water surface will again be specified by a user given factor times the wind speed times the timestep. The user has to take notice of the fact that it is not allowed to create or use WAQUA fields with wind involved, if those fields are used in a later stage in cyclical calculations of a SIMPAR simulation.

1.9 Momentaneous sources and continuous sources

A simulation with SIMPAR can be based on momentaneous sources as well as continuous sources. Momentaneous sources are the ones where all particles are released simultaneously. Continuous sources are characterised by a continous release of particles during a certain time period, which may vary in intensity.

1.10 Geographical aspects

The position of the sources is represented by geographical coordinates (x,y) with Paris as point of reference. In SIMPAR these coordinates are transformed to model (n,m) coordinates. The transformation to spherical coordinates is not yet implemented.

1.11 Release of particles in the environment

1.11.1 Source or group

Particles are released in groups. From a certain geographical position more than one group of particles might be released. One group may contain a variable number of particles.

1.11.2 Particle property

SIMPAR has arrays (PROPAR and GRPROP) in which the physical and chemical properties of the particles are stored. Only mass is implemented as a particle propery, other properties can de added.

1.12 Mass disintegration

With the introduction of particle properties in SIMPAR, it is possible to take mass disintegration into account. Mass (*m)* is defined as a particle property. The initial property value (the mass) must be given by the user and also the rate of disintegration is given by the user by means of the TCHAR keyword. (see User Input)
The disintegration itself is an exponential decrease,

$$m = m_0 \; e^{-tchart}$$

where a small value for TCHAR means fast disintegration and a high value means slow disintegration. TCHAR = 0 means no disintegration at all.

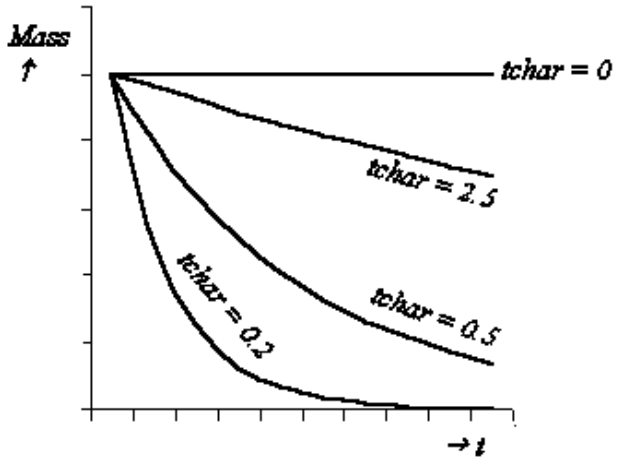


Illustration of mass disintegration

Furthermore it is possible to define more than one property.
I.e. a second property can be defined which represents the temperature. Each property has its own rate of disintegration.

NOTES

- The properties are specified groups wise. So each particle group has its own properties with the corresponding rates.
- When defining more than one property the first property (property with sequence number 1) has to be the mass.
- SIMPAR keeps record of the properties through their sequence number. Therefore in case of multiple properties, the user himself has to keep in mind what each property stands for.
- It is not allowed to use a negative rate of disintegration. A negative value would imply increase rather than decrease, which is not the

intention of the disintegration functionality. So TCHAR should always be at least zero.
- In case of mass disintegration, the use of continuous sources is prohibited.

1.13 Concentration

Besides particle tracks and mass disintegration, SIMPAR can also make concentration calculations.

1.13.1 Concentration grid

The concentration calculations are made on a subgrid, the so called total concentration grid (G1) completely independent on the (curvilinear) WAQUA grid, as illustrated in figure 5 and 6.
The concentration grid is laid on the rectangular area, where the small square grid space size CELLDX in meters is chosen, and the number of grid spacves in the two dimensions, CONLEN and CONWID, are chosen. The grid direction for CONLEN from left to right corresponds to the x-RD-direction. The upward direction for CONWID corresponds to the y-RD-direction.

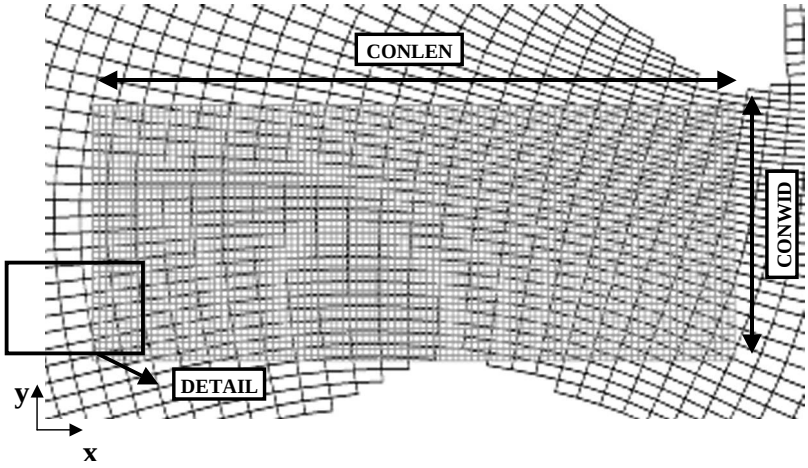


Fig. 5 Overview of the total concentration grid G1

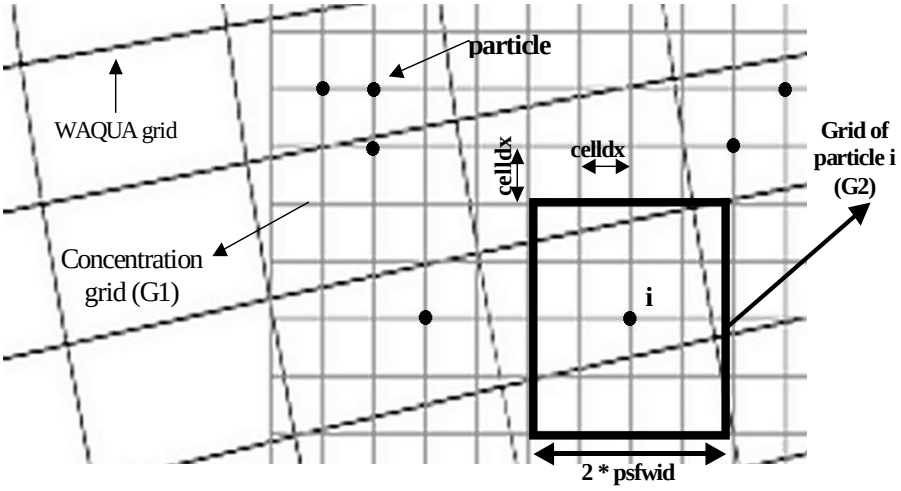


Fig. 6 Overview of the structure of the grid G2(i) for particle I where the spread function is defined. Each particle lies in the center of its own G2(i). The particle positions are rounded to the bottm left corner of the small squares of G1.

These concentration profiles can be calculated by using histogram-like functions or by using pointspread functions. The user can choose to run a simulation with histograms, with pointspread functions or without any concentration profiles. This choice is made by means of the keyword IPSF (see User Input).

1.13.2 Pointspread function method

But because the "exact physical" coordinates of the particles are known, it is beneficial to use these. Therefore the concentration calculations are made on the concentration grid (see 1.13.1).
This concentration grid is based on the particle positions of the current time. Because this concentration grid is based on the particle positions, it has no fixed size. As the cloud of particles can change every time-step, the size of the concentration grid may also change. For each timestep SIMPAR keeps record of the concentration gridsize.

Pointspread functions spread the mass of a particle across neighbouring gridcells, wich results in a much smoother and more accurate concentration than when using histograms.

1.13.3 Histogram method

The histogram method is the simplest method for the concentration calculations. With the histogram method the number of particles withtin a grid cell is counted. This number is than divided by the cell surface to get a rough estimate for the concentration.
Problems arise with the curvilinear grid: the gridcells are often too large for accurate concentration calculations, and the surface of a cell is not necessearily easy to calculate. In this situation or when a more accurate concentration is wanted the histogram method is not very useful.

1.13.4 Total concentration

The concentrations that are saved to the SDS file are average concentrations. When using concentration calculations the user has to define certain input variables, such as the size of the concentration grid and the size of a concentration gridcell. Also the user can define the start time, the interval time, and the end time for the concetration calculations.

NOTES

- The use of concentration profiles implies that the initial mass is known. Thus, when using concentrations the initial mass has to be given by means of keyword **GRPROP** (see § 1.11.2).
- The concentrations functionality can be used in combination with mass disintegration. If only concentrations are required and no mass disintegration the keyword **TCHAR** has to be set to zero.
- Continuous sources may not be used in combination with concentrations!

For more detailed information about concentration profiles see the report “Extension of SIMPAR with Pointspread Functions” (cf. Ref. J.W. Stijnen, H.X.Lin (2000))

1.14 Output results

It is possible to store in file the whole particle field which is generated at some point of time. Also a tracking option exists, i.e. to follow in time with another frequency a selected number of particles.

NOTE

For the calculation of the displacement of a specific particle from a specific point in time, the **next** available velocity of water movement, waterlevel and geometry will be used. So, when WAQUA data at times T0 en T1 are available and the particle leaves at time t_d ($T0 < t_d < T1$), the displacement is calculated based on the data at time point T1.

2 Input description of SIMPAR

2.1 General information

The input is based on SIMONA KEYWORD structure. Refer to "About SIMONA" in Section 1 "General Information".
Reminder: The input file is a structured ASCII-file. From the input file only the first 120 columns are read.

Note: *If the last keyword block in the input file contains a sequential keyword, the SIMONA application independent preprocessor is not able to check the correctness of the block. This can result in incorrect processing of the input file!*

2.1.1 Conventions used

For the input definition the following conventions are used:

[val]	:	real value[1]
[tval]	:	time specification in the form: *day hours:minutes* (e.g. 2 21:15). Times are given relative to midnight of a reference date, starting at 0 0:00.
[ival]	:	integer value
[iseq]	:	sequence number to indicate a point, curve, etc.
[text]	:	string (enclosed between quotes)
< ... >	:	repetition group
| A		
<	:	choice between A and B (A and B are mutually exclusive)
| B		
&	:	continuation mark

In this document keywords are partly underlined (e.g., PRINTOUTPUT). Only the underlined characters are significant. So the user must type at least PRINT in his input, but PRINTOUT is accepted as well.

The 'Explanation' part of the description of the various sections and subsections is divided in three columns:

KEYWORD **E** Explanation

E can be O, M, D, S, R, X.

O means keyword is optional.

M means keyword is mandatory.

D means keyword has a default value. When this keyword is omitted, the pre-processor will use the default value for the variable specified by means of this keyword.

S means this keyword is a sequential keyword: a keyword followed by an integer (e.g. P4). A sequential keyword can be used repeatedly.

R means keyword may occur more than once.

X Exactly one of a series of keywords should be given.

[1] Since all values are read in free format: integer notation (when reals are expected) will be converted to reals, so "val = 4" is identical to "val = 4.0".

2.1.2 Data fields

Data field input is to be specified in two blocks:

```
SPACE_VARYING_DATA
   GLOBAL
   LOCAL
```

SPACE_VARYING_DATA stands for any key-word representing spatial data. In GLOBAL the data for the complete field is to be given, specifying function values at all grid points. In LOCAL however the user can specify rectangular boxes in which he can change the value of the space varying data. For the case of 3D this definition is extended in such a way that the input for separate layers is possible.

2.1.2.1 GLOBAL

Global data can be specified in two ways: first by giving one value for the complete computational grid, second by giving values for each grid point. The order in which these values are to be given is specified by the layout flag.

```
GLOBAL
   LAYOUT = [ival]
   |  CONST_VALUE = [val]
   <
   |  VARIABLE_VALUES = < [ival] >
```

Explanation:

LAYOUT = *[ival]* **D** Layout-indicator specifying the order in which the values from input file are assigned to the function value in a grid point. Possible values for LAYOUT and their meaning are:[2]

1. function values at grid points: $[(m_1,n_1), (m_1,n_1+1) \ldots (m_1,n_2)]$, $[(m_1+1,n_1) \ldots (m_1+1,n_2)] \ldots [(m_2,n_1) \ldots (m_2,n_2)]$
   columns; first column is left; column values from bottom to top
2. function values at grid points: $[(m_1,n_1), (m_1+1,n_1) \ldots (m_2,n_1)]$, $[(m_1,n_1+1) \ldots (m_2,n_1+1)] \ldots [(m_1,n_2) \ldots (m_2,n_2)]$
   rows; first row is bottom; row values from left to right
3. function values at grid points: $[(m_2,n_1), (m_2,n_1+1) \ldots (m_2,n_2)]$, $[(m_2-1,n_1) \ldots (m_2-1,n_2)] \ldots [(m_1,n_1) \ldots (m_1,n_2)]$
   columns; first column is right; column values from bottom to top
4. function values at grid points: $[(m_2,n_1), (m_2-1,n_1) \ldots (m_1,n_1)]$, $[(m_2,n_1+1) \ldots (m_1,n_1+1)] \ldots [(m_2,n_2) \ldots (m_1,n_2)]$
   rows; first row is bottom; row values from right to left
5. function values at grid points: $[(m_1,n_2), (m_1,n_2-1) \ldots (m_1,n_1)]$, $[(m_1+1,n_2) \ldots (m_1+1,n_1)] \ldots [(m_2,n_2) \ldots (m_2,n_1)]$
   columns; first column is left; column values from top to bottom
6. function values at grid points: $[(m_1,n_2), (m_1+1,n_2) \ldots (m_2,n_2)]$, $[(m_1,n_2-1) \ldots (m_2,n_2-1)] \ldots [(m_1,n_1) \ldots (m_2,n_1)]$
   rows; first row is top; row values from left to right

[2] Assume the limits of the box are given by (m_1, n_1) and (m_2, n_2) with $m_1 \leq m_2$ and $n_1 \leq n_2$. In the case of global input $n_1 = 1$, n_2=NMAX, $m_1 = 1$ and m_2= MMAX. The number of required function values is then $n_{tot} * m_{tot}$, where :
n_{tot}= (number of enclosed n grid points) = $n_2 - n_1 + 1$
m_{tot}= (number of enclosed m grid points) = $m_2 - m_1 + 1$

7. function values at grid points: [(m_2,n_2), (m_2,n_2-1) ... (m_2,n_1)], [(m_2-1,n_2) ... (m_2-1,n_1)] ... [(m_1,n_2) ... (m_1,n_1)]
   columns; first column is right; column values from top to bottom
8. function values at grid points: [(m_2,n_2), (m_2-1,n_2) ... (m_1,n_2)], [(m2,n2-1) ... (m1,n2-1)] ... [(m2,n1) ... (m1,n1)]
   rows; first row is top; row values from right to left

Default = 1.

CONST_VALUES = *[val]* **O** Constant value for the complete field.
Default = 0.

VARIABLE_VALUES = < *[val]* > **O** It is possible to specify a function value at each grid point . The order in which the values are to be given is defined by means of layout-indicator.
In the case of 3D the information must be specified as a set of KMAX separate layers, each layer given according to the global layout-indicator (i.e. MMAX*NMAX*KMAX values must be specified, beginning with the top layer) .

2.1.2.2 LOCAL

In LOCAL the function values at grid points specified in GLOBAL can locally be overwritten by specifying boxes (i.e. rectangles). In the 3D-case a box is a rectangle drawn in the horizontal plane identified by the layer-index.

```
LOCAL
  < BOX: MNMN = ( [ival], [ival] ) ( [ival], [ival] ) LAYER = [ival]
      | CONST_VALUES = [val]
    <
      | CORNER_VALUES = [val], [val], [val], [val]
    <
      | VARIABLE_VALUES = < [val] >
```

Explanation:

BOX **R** A BOX is defined by specifying its opposite corner points (m1,n1) and (m2,n2), where m1 ≤ m2 and n1 ≤ n2. In this rectangle the global function value of a "field" variable can be overwritten by new values. It is possible to define more than one box for one single "field" variable. When the rectangles defined in the boxes have common grid points, the latest values specified for those grid point will be used.
The data can be specified either by means of a single value defining all points within the box or by means of a array of data. In the latter case the data should be given according to the following scheme:

MNMN = *([ival], [ival]) ([ival], [ival])*
M Corner points of the rectangular box, specifying (m_1, n_1) (m_2, n_2), where m1 ≤ m2 and n1 ≤ n2.

LAYER = *[ival]* **O** Layer index , where 0 ≤ layer ≤ kmax. If layer is not specified or layer=0, a uniform vertical distribution is assumed. However, when the function values belong to a data-array which is defined for layers 0 until kmax, layer=0 is only valid for the upper layer

and layer=-1 will define the uniform vertical distribution. As default, 3D-arrays are assumed to be defined for layers 1 until kmax, unless stated otherwise in their input description. LAYER is only relevant in the 3D-case.

CONST_VALUES = *[val]*

- The function at all grid points in the box gets this value.

CORNER_VALUES = *[val], [val], [val], [val]*

- The function values at the corner points of the box are given in the following order (m_1, n_1), (m_2, n_1), (m_2, n_2), (m_1, n_2). The function values at the other grid points enclosed by the box will be determined by means of bilinear interpolation.

VARIABLE_VALUES = < *[val]* >

- Inside the box for each grid point a function value is specified. The order in which the values are to be given is set by LAYOUT under key-word GLOBAL.

For example:

```
GLOBAL
   CONST_VALUES = 40.5
   LAYOUT = 4
LOCAL
   BOX:  MNMN = (10, 5), (50, 100)
         CONST_VALUES = 38
```

or

```
GLOBAL
   CONST_VALUES = 0
   LAYOUT = 3
LOCAL
   BOX:  MNMN = (10, 5), (11, 7)
         VARIABLE_VALUES =  2  2.3   2.4
                           1.9   2.0   3.2
```

3 The Input File of SIMPAR

The input of the SIMPAR program is described in this chapter.

3.1 General Information

For general information about the conventions being used for the data fields the reader is referred to section 2.1.1 of this user's guide.

3.2 Echo

The first statement in the input file may set the echo environment. This means that the contents of the input file will or will not be sent to the user's standard output (in general: the message file).

SET NOECHO Tell SIMPAR that no echo of input file contents is needed.

3.3 Warnings

The number of warnings in the message file may be restricted to a user defined number. Default is 10.

SET MAXWARN Sets the number of warnings in the message file.

3.4 Main keywords

The input is divided into 4 main keywords

PARTICLES (Mandatory)

SDSNAMES (Mandatory)

RESTART (Optional)

OUTPUT (Optional)

These keywords are described in the following sections.

3.4.1 PARTICLES (mandatory)

Main keyword **PARTICLES** covers several KEYWORDs that has to be given as initial values to the SIMPAR-simulation by the user. Together these KEYWORD values control the behavior of the SIMPAR simulation model.

PARTICLES **M** There are nine subgroups related to particles.

```
PARTICLES    (M)
   INTEGERS  (M)
   REALS     (M)
   SOURCES   (O)
   NUMBERS   (O)
   TRACKS    (O)
   TIMES     (M)
   WIND     (O)
   CONTSRCS  (O)
   DIFFUSION (O)
```

3.4.1.1 INTEGERS (mandatory)

INTEGERS **M** There are 17 integer input variables.

```
INTEGERS
   NDIM   = [ival]
   IMODEL = [ival]
   IBCK   = [ival]
   ITPAR  = [ival]
   NPARG  = [ival]
   ISTEP  = [ival]
   NPTRAC = [ival]
   IMOVE  = [ival]
   IFIELD = [ival]
   IVELO  = [ival]
   DATIME = [ival]
   IHURST = [ival]
   MEMO   = [ival]
   CONLEN = [ival]
   CONWID = [ival]
   IPSF   = [ival]
   PDIM   = [ival]
```

NDIM=*[ival]* **D** Specifies the model dimension.
For WAQUA: 2
For TRIWAQ: 3
For the time being SIMPAR can only handle 2.
Default = 2

IMODEL=*[ival]* **D** Specifies the type of model that is used for the transport of particles:

1 = floating particle transport
2 = dissolved particle transport
3 = suspended particle transport (not yet implemented)
Default = 1

IBCK=*[ival]* **D** Specify = 1, if backtracking (reverse in time) should be done.
Only allowed if:
floating particle transport (IMODEL = 1)
advection only (IMOVE = 1)
no cyclic velocity fields (IVELO ≠ 3)
no restart(s)
Default = 0

ITPAR=*[ival]* **D** Specifies the maximum number of iterations executed per time step and per particle. It is recommended to use the value 2.
Default = 3

NPARG=*[ival]* **O** Specifies the number of particle groups.
It's equivalent to the number of momentaneous sources. It does not include the number of continuous sources.
Default = 0

ISTEP=*[ival]* **D** Is an indicator related to the calculation of the time step:

0 = user defined (fixed) time step
1 = program determines time step (not implemented)
Default = 0

NPTRAC=*[ival]* **D** Specifies the number of particles that will be tracked.
Subsequently for NPTRAC particles the status of each distinct particle, the group number of the particle and the serial number must be specified.
Default = 0

IMOVE=*[ival]* **M** Specifies the type of particle-movement.

1 = only advection
2 = advection and diffusion

IFIELD=*[ival]* **D** Specifies the kind of wind field.

0 = No extra wind in SIMPAR even if the user had specified wind.
1 = In case of floating particles, global WAQUA-wind or space varying wind in SIMPAR. In case of cyclic fields, a user defined wind.
Default = 0

Note: In case of space varying wind, the wind SDS filename and the experiment name of the wind SDS must be specified (see 3.4.1.10)

IVELO=*[ival]* **D** Specifies which kind of velocity field has to be selected.

1 = momentaneous WAQUA-velocity fields
2 = integrated Eulerian rest-current fields
3 = cyclic velocity fields based on momentaneous WAQUA-velocity fields
Default = 2

Note: when ivelo = 3, no restarts (see 3.4.3) are allowed.

DATIME=*[ival]* **D** Specifies the method of time specification.

1 = All times are specified relative in relation to the start time of WAQUA in elapsed minutes after midnight.
2 = All times are specified in an absolute sense.
Default = 1

IHURST=*[ival]* **D** Indicator for type of diffusion.
1 = Random walk
2 = Fractional Brownian motion.
Default = 1

MEMO=*[ival]* **D** Memory of the fractional Brownian motion.
Default = 100

CONLEN=*[ival]* **D** Maximal length of the concentration grid.
Default = 1000

CONWID=*[ival]* **D** Maximal width of the concentration grid.
Default = 1000

IPSF =*[ival]* **D** Type of pointspread function.
1 = psf
2 = histogram method
3 = no concentrations
Default = 3

PDIM=*[ival]* **D** Number of particles properties. The first property always represents mass. PDIM should be at least one. In other words the mass property is always present.
Default = 1

3.4.1.2 REALS (mandatory)

REALS **M** There are 19 real input variables.

```
REALS
   TSTEP  = [val]
   TIPARW = [val]
|  TFPARW = [val]
|  TLPARW = [val]
<
|  DATFPW = [val]
|  TIMFPW = [val]
|  DATLPW = [val]
|  TIMLPW = [val]
   PARAA  = [val]
   PARAB  = [val]
   PARAC  = [val]
   WOPFAC = [val]
   TITRAC = [val]
|  TFTRAC = [val]
|  TLTRAC = [val]
<
```

```
|  DATFTW = [val]
|  TIMFTW = [val]
|  DATLTW = [val]
|  TIMLTW = [val]
   CELLDX = [val]
   PSFWID = [val]
   HURST  = [val]
   TFCONC = [val]
   TFCONC = [val]
   TLCONC = [val]
```

TSTEP=*[val]* **M** Specifies the time step that is used for SIMPAR simulations. During the simulation process SIMPAR adapts time steps constantly to output requirements: SIMPAR synchronizes those time intervals in a sense that output is always available when it is needed. So, there is no need for interpolation between two intervals.

TFPARW, TIPARW and **TLPARW** specify writing times to disk of particles positions relative to the start of the WAQUA-simulation, respectively first time, time interval and when to write last. **DATIME** must have a value of 1 in this case, explicitly or by default.

TFPARW=*[val]* **O** Specifies the first writing time of particle positions relative to the start of the simulation.

TIPARW=*[val]* **M** Specifies the time interval of writing.

TLPARW=*[val]* **O** Specifies the last writing time of particle positions relative to the start of the simulation**.**

As an alternative the user also can specify absolute datum's and times. **DATFPW** and **TIMFPW**, **DATLPW** and **TIMLPW** are in time/date format and specify when all particles positions must be written to disk for the first time and when last. **DATIME** must have a value of 2 in this case.

DATFPW=*[val]* **O** Specifies the starting date of writing; format *yyyymmdd*.

TIMFPW=*[val]* **O** Specifies the absolute starting time of writing; format *hhmmss*.

DATLPW=*[val]* **O** Specifies the date when to finish writing; format *yyyymmdd*.

TIMLPW=*[val]* **O** Specifies the absolute time when to finish writing; format *hhmmss*.

PARAA=*[val]*, PARAB=*[val]*, PARAC=*[val]* D

PARAA, PARAB and **PARAC** specify the standard deviation of the random displacement of a particle in respectively the horizontal velocity direction, in a velocity direction perpendicular to this direction in the horizontal plane, and in the vertical direction. It can be interpreted as an XYZ-system or a 3-dimensional system. The vertical direction is not yet operational. (As an indication of magnitude the WAQUA diffusion coefficient may be selected.)
Default **PARAA** = 0.
Default **PARAB** = 0.
Default **PARAC** = 0.

WOPFAC=*[val]* **D** Specifies the influence of wind in conjunction with floating constituents. The wind factor is a percentage constant that represents an additional displacement of floating constituents caused by wind.
Default **WOPFAC** = 0.

TFTRAC, **TITRAC** and **TLTRAC** specify the points in time at which the positions of the particles that have been tracked, should be written to disk. **DATIME** must have a value of 1 in this case, explicitly or by default.
When **NPTRAC** > 0 and **DATIME** = 1, **TFTRAC**, **TITRAC** and **TLTRAC** must be specified.

TFTRAC=*[val]* **O** Specifies the starting time point of particles tracking in minutes after the start of the simulation**.**

TITRAC=***[val]*** **O** Specifies the time interval in minutes.

TLTRAC=***[val]*** **O** Specifies the time when to finish particles tracking in minutes after the start of the simulation.

As an alternative the user also can specify absolute datum's and times. **DATFTW** and **TIMFTW, DATLTW** and **TIMLTW** are in date/time format and specify when all tracking positions have be written to disk for the first time and when at last. **DATIME** must have a value of 2 in this case.
When **NPTRAC** > 0 and **DATIME** = 2**, DATFTW**, **TIMFTW**, **TITRAC**, **DATLTW** and **TIMLTW** must be specified.

DATFTW=***[val]*** **O** Specifies the starting date of tracking; format *yyyymmdd.*

TIMFTW=*[val]* **O** Specifies the absolute starting time of tracking; format *hhmmss.*

DATLTW=*[val]* **O** Specifies the date when to finish tracking; format *yyyymmdd.*

TIMLTW=*[val]* **O** Specifies the absolute time when to finish tracking; format *hmmss.*

CELLDX=*[val]* **D** Specifies the size of the concentration gridcell. Should be smaller than the size of the normal gridcell.
Default = 100.0.

PSFWID =*[val]* **D** Specifies the half width of the pointspread function. The width of the pointspread function (2 * psfwid) should be greater than the concentratin gridsize.
Default = 300.0.

HURST=*[val]* **D** Specifies the Hurst factor. Must be between 0 and 1.
When ½ < hurst factor < 1, the motion is *persistent.*
For hurstfactor = 0.5, we have the random walk movement.
When 0 < hurst factor < ½ , the motion is *anti-persistent.*
This parameter needs only to be set if IHURST = 2.
Default = 0.5.

TFCONC=*[val]* **O** Specifies the starting time for particle position output.

TICONC=*[val]* **O** Specifies the interval time for particle position output.

TLCONC=*[val]* **O** Specifies the end time for particle position output.

3.4.1.3 SOURCES (optional)

SOURCES **O** The next KEYWORD is **SOURCES**. It specifies for each distinct momentaneous group (**NPARG**), where the origin in model coordinates is situated. The number of groups of sources must be equal to **NPARG**.

```
SOURCES
   < XYZCRD = ([val], [val], [val]) >
```

XYZCRD=(*[val],[val],[val]*) **M** Specifies the position of the momentaneous sources, in meters relative to Paris. **NPARG** must be greater than 0.

For example, in case **NPARG** = 2:

```
SOURCES
   XYZCRD=( 51250.00, 405750.00, 25.)
   XYZCRD=( 51150.00, 405700.00, 20.)
```

3.4.1.4 NUMBERS (optional)

NUMBERS **O** By means of KEYWORD **NUMBERS** the user specifies the number of particles that participates in each distinct momentaneous group. This is done by indicating two numbers : first the group number and second the number of particles that belongs to that group.

```
NUMBERS
   <GROUP[iseq] : [ival]>
```

GROUP *[iseq]:[ival]* M By means of **GROUP** the group number is specified.

3.4.1.5 TRACKS (optional)

TRACKS **O** If the user wants to activate the tracking of particles, he/she can do this by means of the KEYWORD **TRACKS.** If **NPTRAC** has been given a value greater than 0, then for **NPTRAC** particles the status of each distinct particle must be specified. This means that per particle the group number and the local number must be given.

```
TRACKS
   < GRELMT[iseq] : [ival] >
```

GRELMT*[iseq]:[ival]* **M** By means of **GRELMT** the user specifies a sequential number of a specific group and the particle number of that group. Groups are numbered sequentially, first all momentaneous sources, followed by all continuous sources.

3.4.1.6 TIMES (mandatory)

TIMES **M** On behalf of **TIMES** the user can specify the start- and stop time of the particle computation.

```
TIMES
  |  COMP  [val, val]
  |  TSTOP_WAQCYCLE = [val]
<
  |  STDATE = [val]
  |  STTIME = [val]
  |  ENDATE = [val]
  |  ENDTIM = [val]
  |  ENDAT_WAQCYCLE = [val]
  |  ENTIM_WAQCYCLE = [val]
```

COMP*[val], [val]* **O** By means of the KEYWORD **COMP** and two points of time, respective start time and end time, the particle computation period is assigned. As an alternative, the user also can specify absolute datum's and times. **STDATE** and **STIME**, **ENDATE** and **ENDTIM** specify respective absolute start time and end time. **DATIME** must have a value of 2 in this case.

TSTOP_WAQCYCLE =*[val]* **O** Specifies the relative end time (elapsed minutes after midnight of the WAQUA-start date) of the WAQUA-cycle in case of cyclic WAQUA-velocity fields (datime = 1 and ivelo = 3, see § 3.4.1.1). Default: last WAQUA-map time.

STDATE=*[val]* **O** Specifies the start date of particle computation; format *yyyymmdd*

STTIME=*[val]* **O** Specifies the absolute start time of particle computation; format *hhmmss.*

ENDATE=*[val]* **O** Specifies the date when to finish particle computation; format *yyyymmdd.*

ENDTIM=*[val]* **O** Specifies the absolute time when to finish particle computation; format *hhmmss*.

ENDAT_WAQCYCLE =*[val]* **O** Specifies the absolute date of the end of the WAQUA-cycle in case of cyclic WAQUA-velocity fields (datime = 2 and ivelo = 3, see § 3.4.1.1). Format *yyyymmdd*.
Default: last WAQUA-map time.

ENTIM_WAQCYCLE =*[val]* **O** Specifies the absolute time of the end of the WAQUA-cycle in case of cyclic WAQUA-velocity fields (datime = 2 and ivelo = 3, see § 3.4.1.1). Format: *hhmmss*.
Default: last WAQUA-map time.

Note 1: The end (date and) time must be greater than the start (date and) time, otherwise an error will be reported and the program stops.

Note 2: At cyclic WAQUA-velocity fields (ivelo = 3, see § 3.4.1.1),

the start time of the WAQUA-cycle is always the same as the start of the SIMPAR-simulation.

The end time of the WAQUA-cycle may be specified by the user (see above). It must fall at or before the last WAQUA-map time. When the end of the WAQUA-cycle is reached, the SIMPAR-simulation continues with WAQUA-velocities situated one step *after* the WAQUA-cycle start time.

3.4.1.7 WIND (optional)

WIND **O** By means of the KEYWORD **WIND** the windaspects are incorporated in the simulation process. Wind is only relevant in case cyclic velocity fields in combination with wind are implemented.

```
WIND
   WSPEED = [val]
   WANGLE = [val]
   WCONVF = [val]
 |   < TIMVAL [val val val] >
<
 |   < WNDVAL [val val val val] >
```

General wind situation.

WSPEED=*[val]* **D** Global wind speed in a dimension specified by WUNIT. See User's guide WAQPRE, § 2.7.3.
Default = 0**.**

WANGLE=*[val]* **D** Global wind direction, in degrees from 0 to 360. Wind direction is measured clockwise from north, where (wind coming from) north equals to 0°, (wind coming from) east equals 90° and so on.
Default = 0**.**

WCONVF=*[val]* **D** Wind conversion factor which is defined by the user.
Default = 1**.**

Wind time series.

From the time given on a certain line until the time given on the next line wind speed and wind angles are specified. Before the first data-line the general wind situation rules. After the last data-line the wind situation lasts until the end of the simulation.

TIMVAL *[val],[val],[val]* **O** Specifies time interval (minutes), **WSPEED** and **WANGLE**. **DATIME** must have a value of 1 in this case.

Example**:**

```
TIMVAL    1000.  1.  90.
TIMVAL    1600.  1.  70.
TIMVAL    2000.  1.  45.
TIMVAL    3000.  1.  90.
```

```
TIMVAL    6000.  1.  00.
TIMVAL    8000.  2.  00.
```

WNDVAL ***[val], [val], [val], [val]*** **O** Specifies absolute date and time, **WSPEED** and **WANGLE**. **DATIME** must have a value of 2 in this case.

Example:

```
WNDVAL    19890320.  164000.  1.  90.
WNDVAL    19890321.  024000.  2.  70.
WNDVAL    19890321.  092000.  2.  45.
WNDVAL    19890322.  020000.  2.  90.
WNDVAL    19890324.  040000.  3.   0.
WNDVAL    19890325.  132000.  2.   0.
```

3.4.1.8 CONTSRCS (optional)

CONTSRCS **O** By means of the KEYWORD **CONTSRCS** the so called continuous sources will be incorporated in the SIMPAR simulation. For each individual group the geographical position, the number of particles released per minute and the start time and stop time of the release have to be specified. The total number of particles released in each continuous group equals **NPART * TIMINT**. Continuous and momentaneous particle sources may be combined in the same SIMPAR simulation. The number of continuous sources is *not* counted in the KEYWORD **NPARG**.

```
CONTSRCS
   < SRC[iseq] >
      DATA
         XYZCRD = ([val], [val], [val])
         NPART  = [ival]
       | TIMINT = [val val]
     <
       | TISSTD = [val]
       | TISSTT = [val]
       | TISEND = [val]
       | TISENT = [val]
```

SRC*[iseq]* **S** Labels each continuous source of particles.

DATA **M** Bundels the data.

XYZCRD=(*[val],[val],[val]*) **M** Specifies the position (x,y,z) of the continuous source in meters, relative to Paris.

NPART=*[ival]* **M** Specifies the number of particles that are to be released per minute.

The user has a choice to specify a start-, stop time and the drain interval of the continuous source. If these times are not specified, the continuous source will be active during the whole computation period specified in KEYWORD **TIMES** (see section 3.4.1.6).
As an alternative, the user also can specify relative times (**TIMINT**, value of **DATIME** must be 1 in this case) or absolute calendar dates and times (**TISSTD**, **TISSTT**, **TISEND** and **TISENT**, value of **DATIME** must be 2 in this case).

TIMINT=*[val] [val]* o Specifies the begin- and end time (in minutes) of the drain interval of the continuous source.

TISSTD =*[val]* o Specifies the start datum of the continuous source draining; format *yyyymmdd*.

TISSTT =*[val]* o Specifies the absolute start time of the continuous source draining; format *hhmmss*.

TISEND= *[val]* o Specifies the end datum of the continuous source draining; format *yyyymmdd*.

TISENT= *[val]* o Specifies the end datum of the continuous source draining; format *yyyymmdd*.

3.4.1.9 DIFFUSION (optional)

DIFFUSION o By means of the keyword DIFFUSION the user may specify diffusion coefficients for SIMPAR. This keyword is only relevant when *dissolved* particle transport is chosen (imodel = 2, see § 3.4.1.1).
When the keyword DIFFUSION is omitted (and imodel = 2) , SIMPAR tries to copy the diffusion coefficients from the WAQUA SDS-file. If not present there, an error message will be printed and the program stops.
In the absence of WAQUA diffusion coefficients the user should here specify the diffusion coefficients for SIMPAR, covering the *whole* computational grid.
When part of the computational grid is covered at keyword DIFFUSION, the remaining (not yet defined) positions are copied from the WAQUA SDS-file. If this fails, also an error message will be printed and program execution stops.
So there is no default value for the diffusion coefficients.

```
DIFFUSION
   GLOBAL
      LAYOUT = [ival]
      |  CONST_VALUES = ([val])
      <
      |  VARIABLE_VALUES = < [val] >
   LOCAL
    < BOX: MNMN = ([ival], [ival] ) ( [ival], [ival] )
      |  CONST_VALUES = [val]
      <
      |  CORNER_VALUES = [val], [val], [val], [val]
      <
      |  VARIABLE_VALUES = < [val] >
    >
```

GLOBAL (mandatory)

Global data can be specified in two ways: first by giving one value for the complete computational grid, second by giving values for each grid point. The order in which these values are to be given is specified by the LAYOUT flag.
Although keyword GLOBAL is mandatory, no value(s) for either CONST_VALUES or VARIABLE_VALUES need to be given for the

diffusion coefficients: missing values will be taken from the WAQUA SDS-file (if present).

Explanation:

LAYOUT = *[ival]*	**D**	See § 2.1.2.1. Default = 1.
CONST_VALUES = *[val]*	**O**	See § 2.1.2.1.
VARIABLE_VALUES = < *[val]* >	**O**	See § 2.1.2.1.

LOCAL (optional)

In LOCAL the function values at grid points specified in GLOBAL can locally be overwritten by specifying boxes (i.e. rectangles).

Explanation:

BOX	**R**	See § 2.1.2.2.
MNMN = *([ival], [ival]) ([ival], ival])*	**M**	See § 2.1.2.2.
CONST_VALUES = *[val]*	**O**	See § 2.1.2.2.
CORNER_VALUES = *[val], [val], [val], [val]*	**O**	See § 2.1.2.2.
VARIABLE_VALUES = < *[val]* >	**O**	See § 2.1.2.2.

3.4.1.10 MASS (optional)

MASS **O** By means of the KEYWORD **MASS** the user can specify for each group the initial property values and the rate of disintegration.

```
MASS
   GRPROP = [val]
   TCHAR  = [val]
```

GRPROP =*[val]* **M** Initial properties for each group. The initial properties have to be specified for each group. Furthermore, the number of particles is given by means of keyword **PDIM**.

TCHAR =*[val]* **M** Property control values (rate of disintegration) for each group. The control values have to be specified for each group and for each property. The control value has to be greater than zero. TCHAR = 0 , means no disintegration.

For example, in case **NPARG** = 2 and **PDIM**=3:

```
MASS
   GRPROP = 100.00 , 250.00, 175.50 ,   (initial properties for group 1)
            450.00 ,  80.00, 800.50     (initial properties for group 2)
   TCHAR  = 0.5 , 1.0 , 1.5 ,     (control values for group 1)
            0.6 , 1.1 , 2.0       (control values for group 2)
```

3.4.2 SDSNAMES (Mandatory)

The second main KEYWORD relates to files. The simulation needs at least **two** SDS files :

- An existing file in which the calculated results of the program WAQUA are stored. Through **WAQSDS** that file is defined. The name of the experiment in the SDS file is given by the **EXPWAQ** keyword.
- The results of the SIMPAR simulation are stored in the SDS file given by the **PARSDS** keyword under the experiment name given by **EXPPAR** If the file does not exist it is created.
- There also exists the option to connect an existing wind SDS file to the SIMPAR simulation model by means of the **WINSDS** and **EXPWIN** keywords.

```
SDSNAMES
   WAQSDS = [text]
   EXPWAQ = [text]
   PARSDS = [text]
   EXPPAR = [text]
   WINSDS = [text]
   EXPWIN = [text]
```

WAQSDS=*[text]* **M** Specifies the underlying, existing WAQUA SDS file. Input file.

EXPWAQ=*[text]* **M** The name of the experiment in WAQSDS.

PARSDS=*[text]* **M** Defines the SDS-file, in which the results of the particle simulation are to be stored.
Output file.

EXPPAR=*[text]* **M** Gives the experiment name under which the calculated data are to be stored in the particle SDS-file.

WINSDS=*[text]* **O** Specifies WAQUA SDS-file with wind data.
Input file.

EXPWIN=*[text]* **O** Name of wind experiment in wind SDS-file.

3.4.3 RESTART (Optional)

The program SIMPAR is provided with a facility to extend the simulation with velocity field data, that originate from another SDS-file, other than the files mentioned in section 3.4.1.10. By means of the KEYWORD **RESTART** the simulation process is directed to act on another SDS file. First the name SDS file is defined, subsequently the name of the experiment and there upon the point of time at which the simulation process must commence. The user is allowed to repeat this procedure several times (maximum = 5). Restart data must be specified with start times in ascending order.

Note: when cyclic WAQUA velocity fields are specified (ivelo = 3, see § 3.4.1.1), restart is *not* allowed.

```
RESTART
   <RES[iseq]>
      WAQSDS = [text]
      EXPWAQ = [text]
    |  TIME  = [val]
   <
    |  RSDATE = [val]
    |  RSTIME = [val]
```

RES*[iseq]* **M** Labels restart actions.

WAQSDS=*[text]* **M** Specifies another WAQUA SDS file

EXPWAQ=*[text]* **M** Experiment name in above mentioned WAQUA SDS file

TIME=*[val]* **O** Start time (min) of restart with respect to the start time of the base run (where **DATIME** = 1)

RSDATE=*[val]* **O** Restart date of a new simulation; format *yyyymmdd* (where **DATIME** = 2)

RSTIME=*[val]* **O** Restart time of a new simulation; format *hhmmss* (where **DATIME** = 2)

3.4.4 OUTPUT (Optional)

Store particle tracking results in an output file.

OUTPUT
  TROUT=*[text]*

TROUT*[text]* **M** Name of the particle tracking output file.

4 Examples

4.1 Example 1

```
#
#   Meld eerst (eventueel) dat U geen echo van alle SIMONA messages op
#   uw scherm wilt :

set noecho

#   Beperk het aantal SIMONA waarschuwingen tot 25. Standaard is 10.

set maxwarn 25

#
#   Het programma kent 4 hoofdkeywords :
#
#   Het eerste hoofdkeywoord is ‘particles’ :

particles

#   ‘particles’ heeft een aantal onderkeywoorden, om te beginnen
#   ‘integers’. In dit blok geeft de gebruiker alle integer
#   constanten waarmee het model wordt gestuurd op :

    integers

#   Met ‘ndim’ wordt de dimensie aangegeven. Voor WAQUA is dat
#   altijd 2 (Voor SIMPAR op dit moment ook)

        ndim   = 2

#   met ‘imodel’ wordt aangegeven welk type model moet worden
#   gebruikt voor de particles :
#    1 betekent drijvend transport
#    2 betekent opgelost transport
#    3 betekent opgewerveld transport (nog niet werkend)

        imodel = 1

#   met ‘itpar’ wordt het aantal iteraties dat maximaal wordt berekend
#   per tijdstap en per particle aangegeven. Geadviseerd wordt om dit
#   op twee te zetten

        itpar  = 2

#   met ‘nparg’ geeft de gebruiker het aantal groepen van deeltjes
#   dat zal worden onderscheiden aan. Het betreft hier de momentane
#   bronnen. Verderop worden de continue bronnen opgegeven.

        nparg  = 1

#   met ‘nptrac’ geeft de gebruiker het aantal deeltjes aan dat
#   zal worden gevolgd i.e. "getrackt"

        nptrac = 7

#   met ‘imove’ geeft de gebruiker het type van de particle
#   beweging aan :
#    1  betekent  alleen advectie
#    2  betekent  advectie en diffusie

        imove  = 1

#   met ‘ifield’ geeft de gebruiker het type windveld aan :
#    0  betekent geen extra wind in SIMPAR, ook al heeft de gebruiker
#       wind gespecificeerd)
#    1  betekent extra standaard WAQUA of TRIWAQ wind in SIMPAR in geval
#       van drijvende stof, of in geval van cyclische velden eigen door
#       gebruiker opgegeven wind

        ifield = 0

#   met ‘ivelo’ geeft de gebruiker aan met welk type snelheidsveld
#   gerekend moet worden :
#    1  betekent momentane WAQUA of TRIWAQ snelheidsvelden
#    2  betekent Eulerse WAQUA of TRIWAQ snelheidsvelden
#    3  betekent periodieke snelheidsvelden gebaseerd op de
#       momentane snelheidsvelden

        ivelo  = 1

#   met ‘datime’ kan de gebruiker opgeven of alle tijden relatief ten
#   opzichte van de starttijd van WAQUA/TRIWAQ in minuten zijn pgegeven
#   datime = 1, (dit is ook de default waarde) of in absolute zin
#   datime = 2
```

```
        datime = 1

#   het volgende keyword is reals :

    reals

#   'tstep' is de tijdstap waarmee het programma zou moeten draaien.
#   het programma past tijdens het proces de tijdstap steeds aan
#   aan de uitvoereisen : is tstep te groot dan wordt tijdelijk met
#   een zodanige stap gerekend dat de uitvoer op de juiste tijdstippen
#   beschikbaar is. Er hoeft dan dus niet geinterpoleerd te worden.

        tstep  =   10.0

#   met 'tfparw', 'tiparw' en 'tlparw' geeft de gebruiker aan wanneer de
#   eerste keer alle particle posities moeten worden weggeschreven,
#   met welk interval daarna en wat het laatste tijdstip van schrijven
#   moet zijn. Ook hier geldt weer dat via 'datfpw', 'timfpw' en
#  'datlpw' en 'timlpw' een alternatief in de vorm van datum en tijd
#   kan worden opgegeven

        tfparw =   4920.
        tiparw =     10.
        tlparw =   5640.
#       datfpw =  19940101
#       timfpw =  060000
#       datlpw =  19940101
#       timlpw =  120000

#   standaarddeviatie van de random verplaatsing op de horizontale
#   snelheidsrichting

        paraa  = 10.

#   standaarddeviatie van de random verplaatsing in de richting normaal
#   op de horizontale snelheidsrichting

        parab  = 10.

#   standaarddeviatie van de random verplaatsing in de verticale
#   richting (nog niet in gebruik)

#       parac  = 10.

#   met de variabele 'wopfac' wordt de invloed van de wind beschreven
#   in het geval van een drijvende stof. De windfactor is een percentage
#   dat de extra verplaatsing ten gevolge van de wind aangeeft voor
#   drijvende stof, op te geven in %

        wopfac = 5

#   met de variabelen 'tftrac', 'titrac' en 'tltrac' wordt aangegeven
#   op welke tijdstippen de posities van de variabelen die getrackt
#   worden, moeten worden weggeschreven.
#   weer hetzelfde alternatief met betrekking tot datum en tijd

        tftrac =   4920.
        titrac =     20.
        tltrac =   5640.
#       datftw = 19940101
#       timftw = 060000
#       datltw = 19940101
#       timltw = 120000

#   het volgende keywoord is 'sources'. Hiermee wordt voor elke
#   groep aangegeven (nparg) waar de oorsprong van de groep ligt

        sources

#   met het woord 'xyzcrd' worden de x,y,z coordinaten gegeven ,
#   van de momentane bronnen :

            xyzcrd = (  51250,  405750, 25. )

#   via het keyword 'numbers' geven we aan dat we op willen geven
#   hoeveel deeltjes in elke momentane groep zitten

        numbers

#   via het keywoord 'groep' en het aantal deeltjes ligt alles vast

            group 1 : 12

#   Met het keyword 'contsrcs' worden de continue bronnen opgegeven.
#   Voor elke groep worden een positie, het aantal deeltjes dat per
#   minuut wordt losgelaten en het lozingsinterval in de tijd opgegeven.

        contsrcs
            src1
                data
```

```
                    xyzcrd = (  51250.00,  405750.00, 25. )
                    npart  = 1
                    timint = 4920. 5640.
#                   tisstd = 19940101
#                   tisstt = 060000
#                   tisend = 19940101
#                   tisent = 120000

#   als er getrackt moet worden geven we dit aan door het
#   keywoord 'tracks' :

        tracks

#   nu volgt voor nptrac deeltjes, welke deeltjes dat precies zijn :
#   per deeltje het groepsnummer en het elementnummer, i.e. het volg-
#   nummer in die groep

            grelmt 1 :   1
            grelmt 1 :   4
            grelmt 1 :   7
            grelmt 1 :   10
            grelmt 2 :   100
            grelmt 2 :   300
            grelmt 2 :   500

#   met het keywoord 'times' geven we aan dat we de begin- en eindtijd
#   van de berekening willen opgeven :

        times

#   via het keywoord 'comp' en de twee tijden voor begin en eindtijd is
#   de rekenperiode vastgelegd :
#   als alternatief kunnen ook de absolute data en tijden worden vastgelegd

            comp  4920 5640
#           stdate   19940101
#           sttime   060000
#           endate   19940101
#           endtim   120000

#   met het keywoord 'wind' wordt de wind gespecificeerd; deze waarden
#   worden alleen gebruikt in het geval van cyclische snelheidsvelden
#   met wind

        wind

#   algemeen :

            wspeed    2.00
            wangle   90.00
            wconvf    2.00

#   specifiek : (vanaf de gegeven tijd tot de eerstvolgende tijd gelden
#                wspeed en wangle zoals hier opgegeven)

    timval    1000.   1.    90.
    timval    1600.   2.    70.
    timval    2000.   2.    45.
    timval    3000.   2.    90.
    timval    6000.   3.     0.
    timval    8000.   2.     0.


#    wndval    19890320.  164000   1.    90.
#    wndval    19890321.  024000   2.    70.
#    wndval    19890321.  092000   2.    45.
#    wndval    19890322.  020000   2.    90.
#    wndval    19890324.  040000   3.     0.
#    wndval    19890325.  132000   2.     0.

# Second main key :

#   de berekening heeft tenminste twee SDS files nodig :
#   1. een file waarop de WAQUA resultaten staan, via WAQSDS wordt die
#   file aangegeven. Via expwaq het experiment op die file.
#   2. via PARSDS en EXPPAR wordt aangegeven op welke SDS file de
#   resultaten zullen worden weggeschreven
#   Er kan ook nog een wind SDS file aangegeven worden.

sdsnames
    waqsds = 'SDS-wkst01'
    expwaq = 'os05'
    parsds = 'SDS-pkst01'
    exppar = 'pkst01'

# Third main key :

#   Het is mogelijk de berekening te laten vervolgen met snelheidsvelden
#   die van een andere SDS file als de start SDS komen. Via het keywoord
#   RESTART wordt dit aangegeven. Eerst wordt de SDS naam genoemd,
```

```
#   vervolgens het experiment en tenslotte de tijd waarop met deze nieuwe
#   file moet worden begonnen. Dit kan, indien gewenst een aantal malen
#   herhaald worden (maximum = 5).

#restart

#  res1
#      waqsds = 'SDS-for.dat'
#      expwaq = 'scaldis400'
#      time   =  1750.
#      rsdate =  19970506
#      rstime =  050000

# Fourth main key :
#   De naam van het 'tracking' uitvoerbestand.

output
    trout = 'pkst01.trk'

# Einde invoer.
```

4.2 Example 2

```
#
# Geen SIMONA messages op scherm
#
set noecho
#
# SIMPAR kent 4 mainkeywords: PARTICLES, SDSNAMES, RESTART en
OUTPUT
# De eerste 2 worden gebruikt, de 3e alleen als er meerdere SDS-
files opgegeven
# zijn en de laatste wordt niet gebruikt.
#
# Het eerste main keyword is particles
#
particles
#
# Particles kent een aantal sub-keywoorden.
# De eerste is integers.
# Hier worden alle integer constanten waarmee het model gestuurd
wordt opgegeven
#
integers
#
#  ndim: aantal dimensies (2 voor waqua)
#
ndim = 2
#
# imodel: model type
# 1 -> drijvend transport
# 2 -> opgelost transport
# 3 -> opgewerveld transport (nog niet operationeel)
#
imodel =   2
#
# itpar: Max. aantal iteraties per tijdstap en per particle.
#
itpar = 2
#
# nparg: aantal momentane bronnen (vast op 1)
#
nparg = 1
#
# nptrac: aantal deeltjes dat getracked wordt
#
nptrac =  250
#
# imove: aard van beweging van de deeltjes
# 1 -> alleen advectie
# 2 -> advectie en diffusie
#
imove =   2
#
# ifield: type windveld
# 0 -> Geen extra wind in SIMPAR
# 1 -> Extra standaard WAQUA wind in SIMPAR
#      (geadviseerd i.g.v. drijvende stof)
#
ifield =   0
```

```
#
# ivelo: type stroomsnelheidsveld
# 1 -> momentane WAQUA snelheidsvelden
# 2 -> Eulerse WAQUA snelheidsvelden
# 3 -> periodieke snelheidsvelden, gebaseerd op de momentane
snelheidsvelden
# Wordt vast op 1 gezet
#
ivelo = 1
#
# datime: tijden relatief t.o.v. starttijd WAQUA (1), of
absoluut (2)
# Wordt vast op 2 gezet
#
datime = 2
#
# Het volgend sub-keyword is reals
# Hier worden alle real constanten opgegeven
#
reals
#
# tstep: de tijdstap waarmee het programma zou moeten draaien.
Het
# programma past tijdens het proces de tijdstap steeds aan aan
de
# uitvoereisen: is tstep te groot dan wordt tijdelijk met een
zo-
# danige stap gerekend dat de uitvoer op de juiste tijdstippen
# beschikbaar komt.
#
tstep = 10.0
#
# Tijdstap berekenen positie deeltjes
#
tiparw = 10.
#
# Begindatum/tijd berekenen positie deeltjes
#
datfpw = 19920929
timfpw =   044000
#
# Einddatum/tijd berekenen positie deeltjes
#
datlpw = 19920929
timlpw =   102000
#
# paraa: standaard afwijking random verplaatsing in X-richting
# parab: standaard afwijking random verplaatsing in Y-richting
# parac: standaard afwijking random verplaatsing in Z-richting
# (wordt niet gebruikt)
# De waarde van deze parameters doet er niet toe:
# hiervoor wordt in SIMPAR de wortel uit de WAQUA diffusie
genomen
#
paraa = 0.1
parab = 0.03
parac = 0.
wopfac =         .00
#
# titrac: tijdstap wegschrijven positie te volgen deeltjes
# datftw: begindatum wegschrijven positie te volgen deeltjes
# timftw: begintijd  wegschrijven positie te volgen deeltjes
# datltw: einddatum wegschrijven positie te volgen deeltjes
# timltw: eindtijd  wegschrijven positie te volgen deeltjes
#
titrac =       10
datftw = 19920929
timftw =   044000
datltw = 19920929
timltw =   102000
#
# Volgende keyword is sources. Hier wordt voor elke bron
aangegeven
# waar de oorsprong ligt.
# Wij gaan uit van 1 momentane bron.
#
sources
#
# x,y,z coordinaten van de momentane bron (z doet niet ter zake)
#
```

```
xyzcrd = (    43550.00,  375100.00, 0. )
#xyzcrd = (    43595.00,  374815.00, 0. )
#
# numbers: keyword om aantal deeltjes op te geven in de
momentane groep
#
numbers
#
# group: er is 1 bron met 250 geloosde deeltjes (vast)
#
group 1 : 250
#
# tracks: keyword dat aangeeft dat er deeltjes gevolgd moeten
worden
#
tracks
#
# Voor nptrac deeltjes opgeven welke deeltjes uit de gehele
groep het
# zijn. Aangenomen wordt dat dit de eerste nptrac deeltjes uit
de
# groep zijn.
#
grelmt 1 :   1
grelmt 1 :   2
grelmt 1 :   3
grelmt 1 :   4
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grelmt 1 : 250
# times: keyword voor aangeven begin- en einddatum/tijd
berekening.
#
times
#
# stdate : begindatum rekenperiode.
# sttime : begintijd rekenperiode
# endate: einddatum rekenperiode.
# endtim: eindtijd rekenperiode
#
stdate = 19920929
sttime =   044000
endate = 19920929
endtim =   102000
#
diffusion
    global
#   layout= 4
    const_value = 50
#
#
# sdsnames: keywoord voor aangeven SDS filenaam
#
sdsnames
#
# Geef naam 1e SDS-file die gebruikt moet worden.
# met experimentnaam
#
waqsds = 'SDS-99'
expwaq = '99'
#
parsds = 'PARTIC'
exppar = 'pasvt'
```

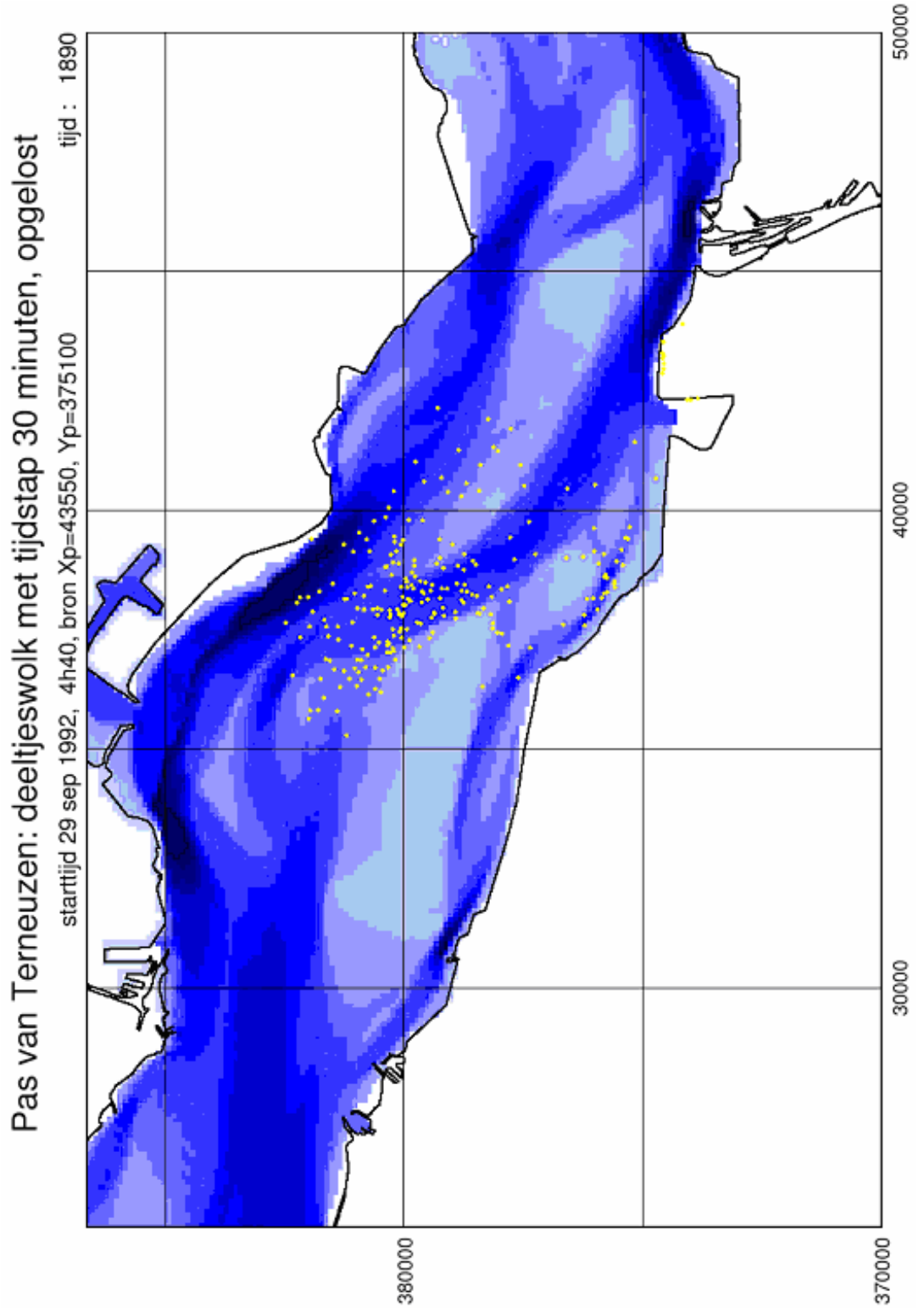
Pas van Terneuzen: deeltjeswolk met tijdstap 30 minuten, opgelost
starttijd 29 sep 1992, 4h40, bron Xp=43550, Yp=375100
tijd : 1890
380000
370000
50000
40000
30000

5 References

- A.W. Heemink (1990)
  1. Stochastic modelling of dispersion in shallow water.
  2. Stochastic Hydrology and Hydraulics, 4, 161-174

- J.W. Stijnen, H.X.Lin (2000)
  1. The Modeling of Diffusion in Particle Models
  2. Extension of SIMPAR with Pointspread Functions

6 Appendices

6.1 List for further reading

User's guide WAQUA.

6.2 Index